Effects of source size and wavefront propagation on the energy resolution of a bent-crystal polychromator

J. P. Sutter, M. Amboage, S. Hayama and S. Díaz-Moreno

Diamond Light Source Proceedings / Volume 1 / Issue MEDSI-6 / October 2011 / e15
DOI: 10.1017/S2044820110000304, Published online: 21 October 2010

Diamond Light Source Proceedings, Vol 1, e15, page 1 of 4
MEDSI-6 2010
doi:10.1017/S2044820110000304

Poster paper

Effects of source size and wavefront propagation on the energy resolution of a bent-crystal polychromator

J. P. SUTTER†, M. AMBOAGE, S. HAYAMA AND S. DÍAZ-MORENO

Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX110DE, UK

(Received 11 June 2010; revised 7 September 2010; accepted 22 September 2010)

Polychromators, or elliptically bent diffracting crystals that focus a broad-bandwidth X-ray beam onto a sample, have become a common device at synchrotron beamlines specializing in X-ray absorption spectroscopy (XAS) because they allow a full absorption spectrum to be collected in one shot. Such a device is being planned for the XAS beamline I20 of the Diamond Light Source. A bent silicon crystal diffracting 7 keV X-rays with the (1 1 1) reflection is taken as a model for the simulations of this report. Instrumental resolution is determined by the demagnification of the source, the spread of the diffracted beam during propagation and the pixel size of the position-sensitive detector placed behind the sample. The first is calculated by geometrical optics. The second is calculated by a full wave-optical treatment, which includes Takagi–Taupin integration to find the diffracted amplitude at the crystal's surface and Huygens–Fresnel propagation of the diffracted wave to the sample or detector. This sets the polychromator's intrinsic energy resolution. The pixel size of the detector is then added to find the total instrumental resolution at various sample–detector distances.

1. Introduction

A bent silicon crystal polychromator that will focus a beam of broad bandwidth onto a sample is being planned for the energy-dispersive branch of the X-ray absorption spectroscopy beamline I20 at the Diamond Light Source. In the following treatment, a bent silicon crystal using the symmetric (1 1 1) Bragg reflection will be modelled. The planned distance between the source and the polychromator is 45.1 m; that between the polychromator and the sample is 1.0 m. A photon energy of 7000 eV is assumed because, at this energy, the absorption and extinction are both high and penetration depth of the radiation is therefore small. The Bragg angle θ_B is thus 16.406° and the radius of curvature R at the centre is 6.9268 m. The expected bandwidth of the polychromator is ±5%. The source at I20 is a wiggler whose horizontal X-ray source size is 590 μm *full width at half-maximum* (FWHM). The position-sensitive detector downstream from the sample has a pixel size of 25 μm.

† Email address for correspondence: john.sutter@diamond.ac.uk

The instrumental energy resolution of the polychromator/detector system is determined by the finite source size, the spread of the wave introduced by diffraction and the pixel size of the detector. See details in Sutter *et al.* (2010) and references therein for discussion and examples at other beamlines.

2. Calculations

The effect of source size on the image size can be seen in figure 1, which displays the 'monochromatic focus' defined by Tolentino *et al.* (1988). Each point P on the elliptical arc that focuses the rays from the central source point S into the central image point F has its own Rowland circle, on which the two monochromatic focal points M_{P1} and M_{P2} are placed. From the central point of the polychromator, the distance to the monochromatic foci is $R \sin \theta = 1.956$ m. The size of the image produced by the rays of wavelength λ_P diffracted in the neighbourhood of P can be found by simple ratios of the distances. If P is the centre of the polychromator, the size of this image will be called S_{dmg}.

However, the wave propagation must also be taken into account. In the following, a spherical wave of photon energy 7000 eV is assumed to be incident on the polychromator. Takagi–Taupin and Huygens–Fresnel theories are used to calculate the diffraction in the crystal and in the free spaces (Sutter *et al.* 2010). Figure 2 shows the resulting diffracted beam spot at various distances d from the polychromator. At the polychromatic focus ($d = 1000$ mm), the diffracted beam is focused to less than 2 μm; $d = 2000$ mm is just beyond the monochromatic focus M_{P2}. Notice the considerable broadening of the beam spot at this point, which removes the advantage of eliminating the source size broadening.

3. Results

Table 1 shows the spot sizes and the contributions to energy resolution coming from the source size, the diffraction and the pixel size. W_{tot} is the sum in

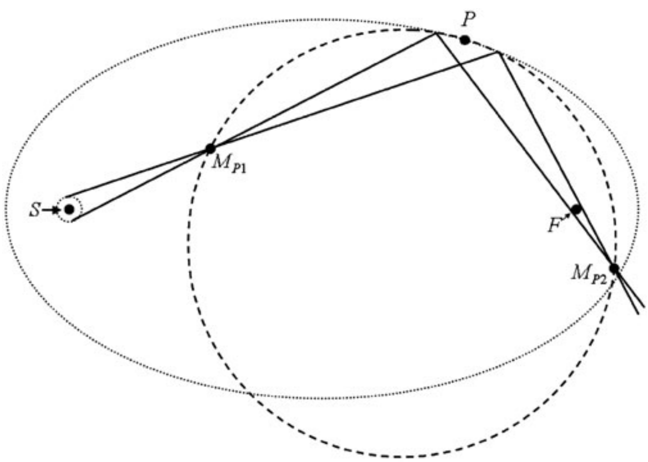

FIGURE 1. Definition of the monochromatic focal points M_{P1} and M_{P2} for a point P on the polychromator that focuses rays from the central source point S into the central image point F.

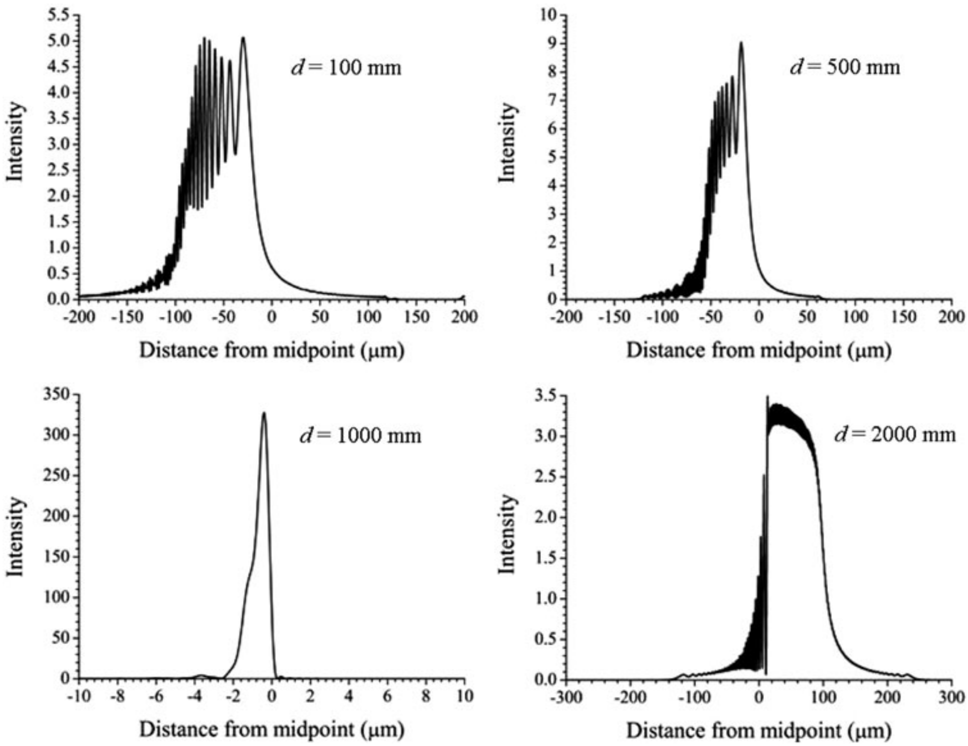

FIGURE 2. Intensity of the diffracted wave at various distances d from the polychromator.

D_{det}, mm	W_{diff}, μm	S_{dmg}, μm	W_{tot}, μm	ΔE_{sp}, eV	ΔE_{pix}, eV	ΔE_{tot}, eV
100	8.3	11.7	14.3	1.66	2.90	3.34
200	16.7	10.3	19.6	1.13	1.45	1.84
300	25.1	9.0	26.7	1.03	0.97	1.41
400	33.6	7.6	34.4	1.00	0.72	1.23
500	42.2	6.3	42.7	0.99	0.58	1.15
600	50.9	4.9	51.1	0.99	0.48	1.10
700	59.4	3.5	59.5	0.98	0.41	1.06
800	67.8	2.1	67.8	0.98	0.36	1.04
900	76.1	0.8	76.1	0.98	0.32	1.03

TABLE 1. Diffraction spot width W_{diff}, demagnified image size S_{dmg}, total broadening W_{tot}, single-point energy resolution ΔE_{sp}, pixel size energy resolution ΔE_{pix}, and total energy resolution ΔE_{tot} as a function of distance D_{det} between detector and polychromatic focus.

quadrature of W_{diff} and S_{dmg}; ΔE_{tot} is the sum in quadrature of ΔE_{sp} and ΔE_{pix}. Note that the energy spread ΔE_{sp} of the waves reaching a single point at the detector falls to a limiting 'intrinsic resolution' of 0.98 eV. The best sample-detector distance is 400–600 mm, where resolution is high and the ray fan small.

REFERENCES

SUTTER, J. P., AMBOAGE, M., HAYAMA, S. & DÍAZ-MORENO, S. 2010 Geometrical and wave-optical effects on the performance of a bent-crystal dispersive X-ray spectrometer. *Nucl. Instrum. Methods Phys. Res.* **A 621**, 627–636.

TOLENTINO, H., DARTYGE, E., FONTAINE, A. & TOURILLON, G. 1988 X-ray absorption spectroscopy in the dispersive mode with synchrotron radiation: optical considerations. *J. Appl. Crystallogr.* **21**, 15–22.